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APPENDIX

APPENDIX A

SPECTRUM OF TETRAZOLE DERIVATIVES

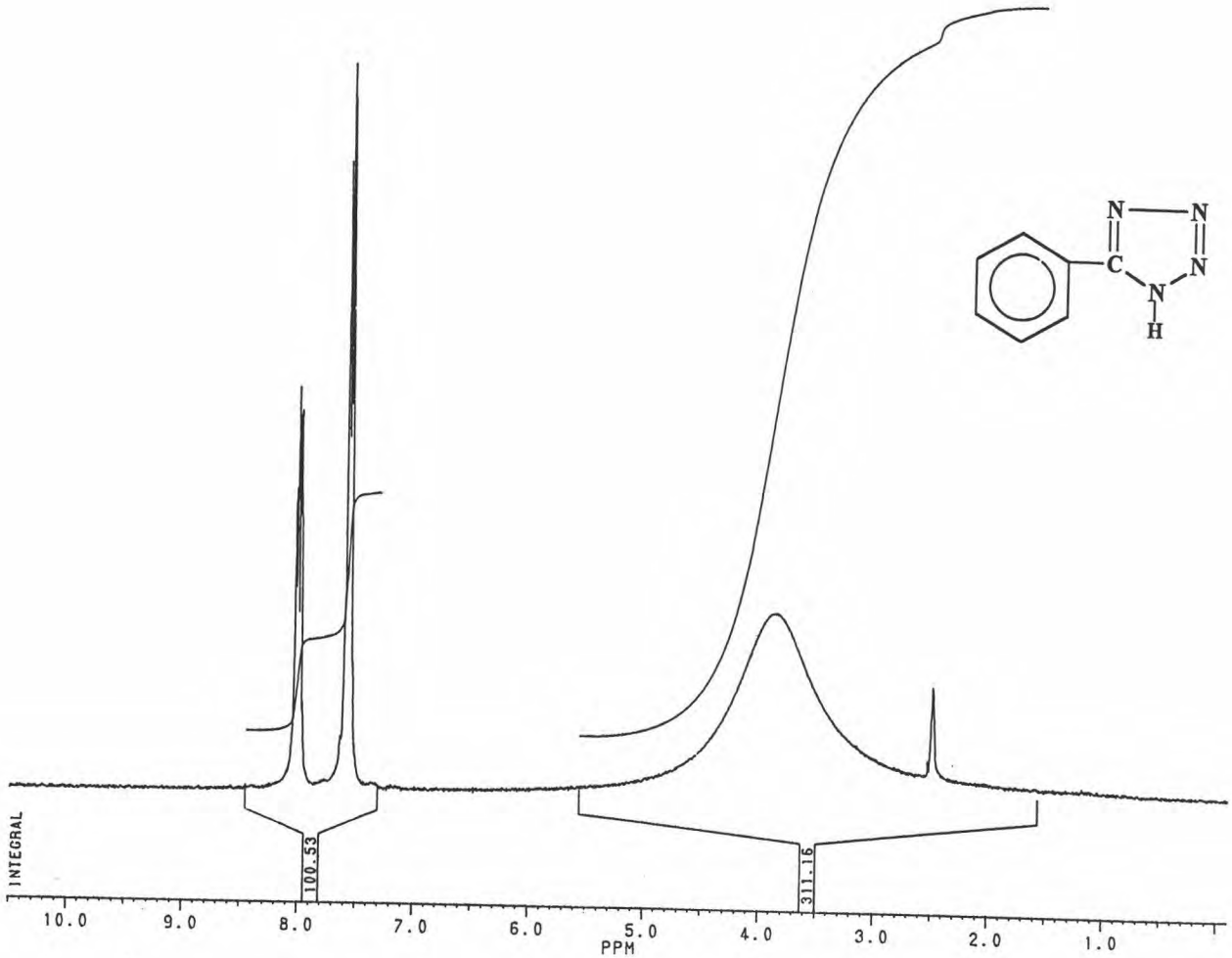

Figure A1 ^{1}H-NMR spectrum (DMSO-d_6) of 5-phenyltetrazole

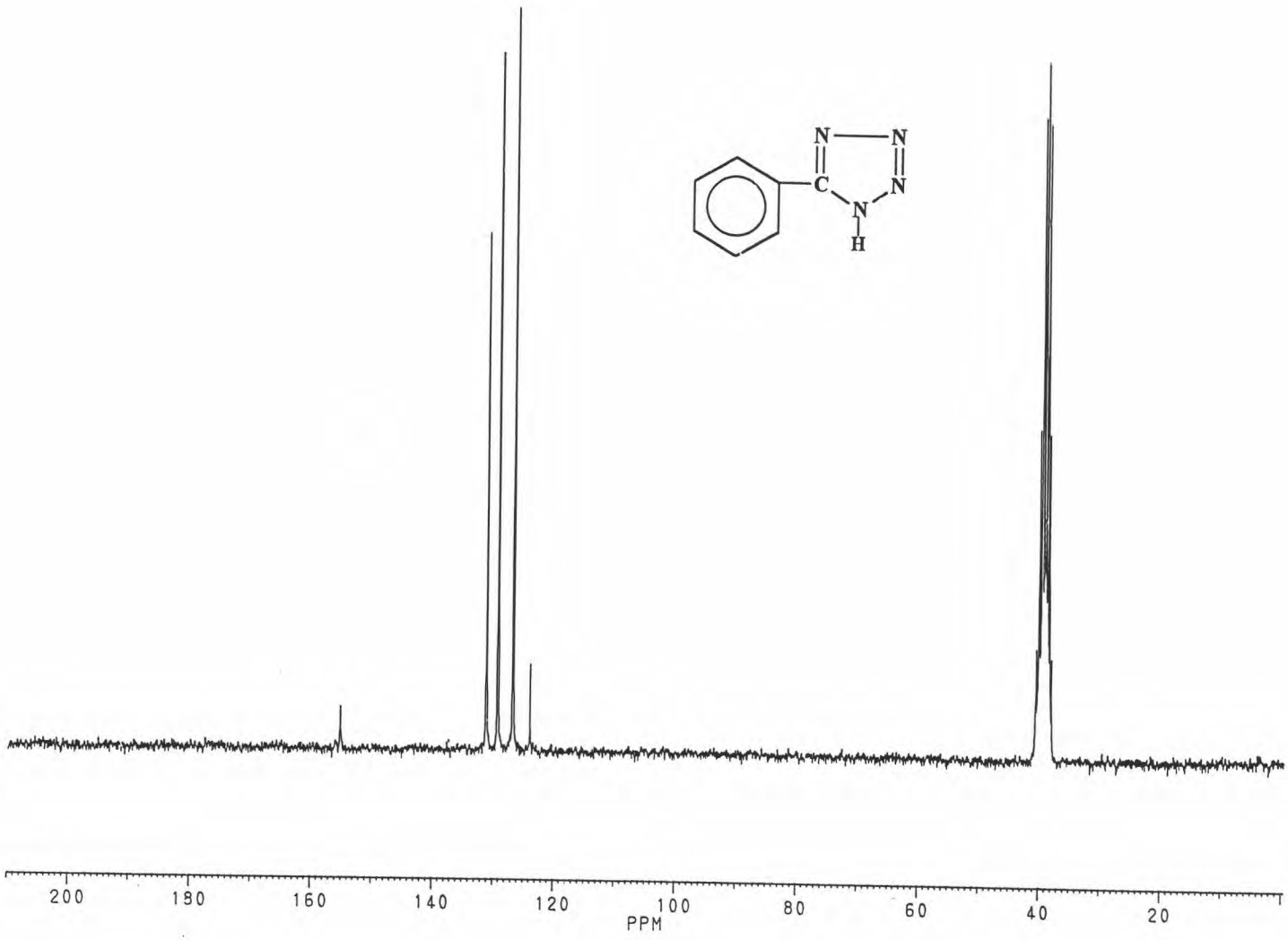

Figure A2 ^{13}C-NMR spectrum (DMSO-d_6) of 5-phenyltetrazole

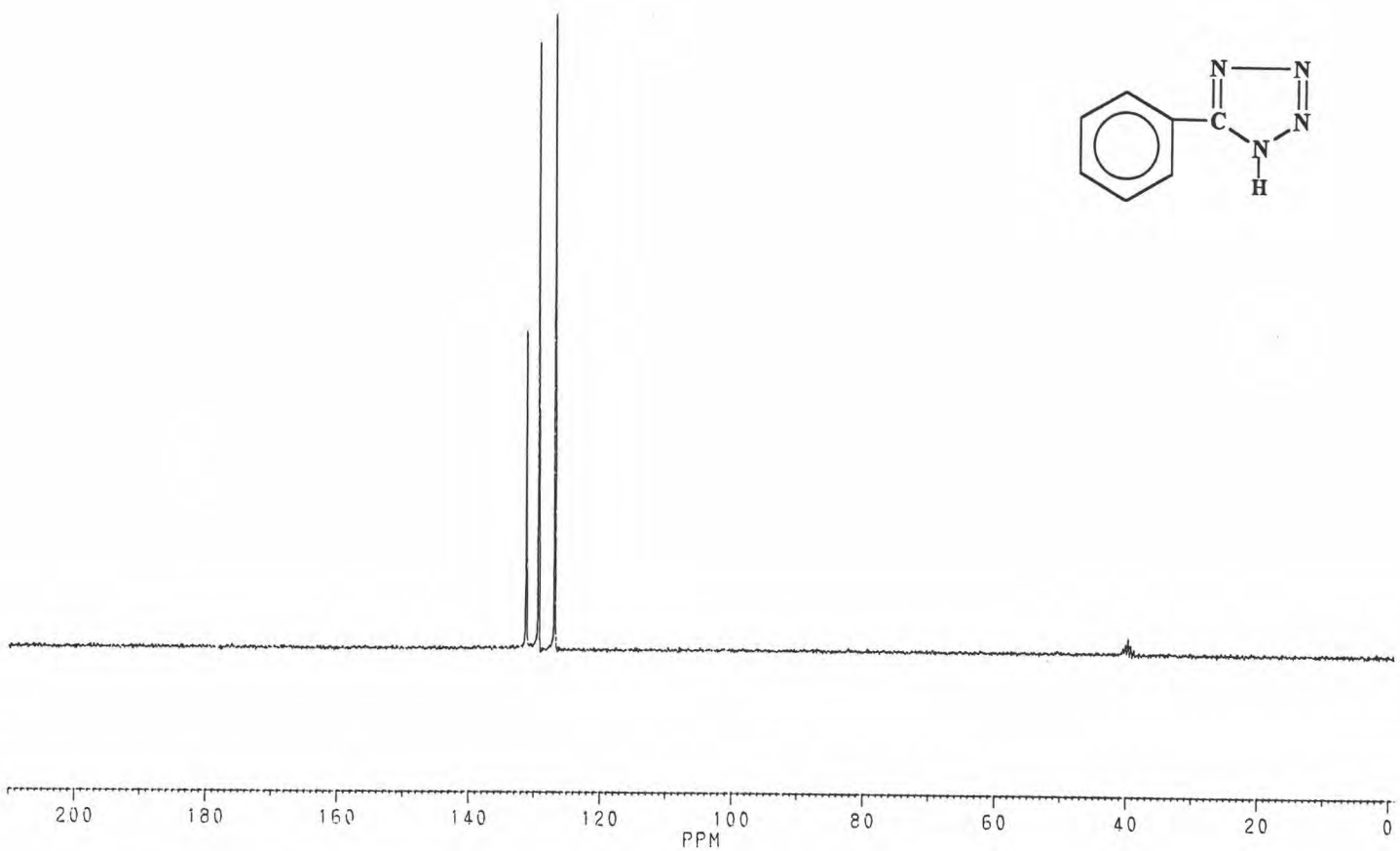

Figure A3 DEPT-90 ^{13}C-NMR spectrum (DMSO-d_6) of 5-phenyltetrazole

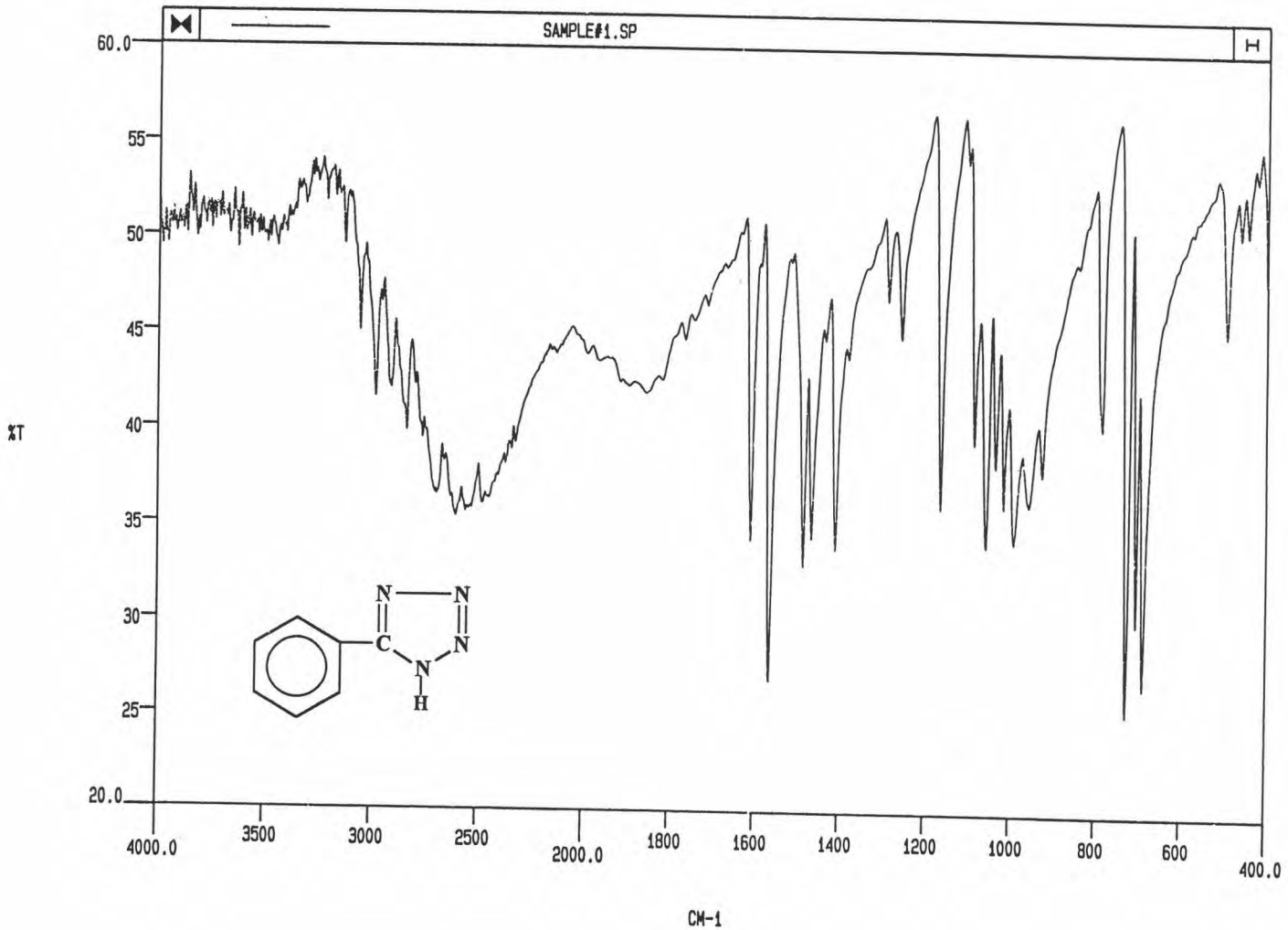

Figure A4 FTIR spectrum of 5-phenyltetrazole

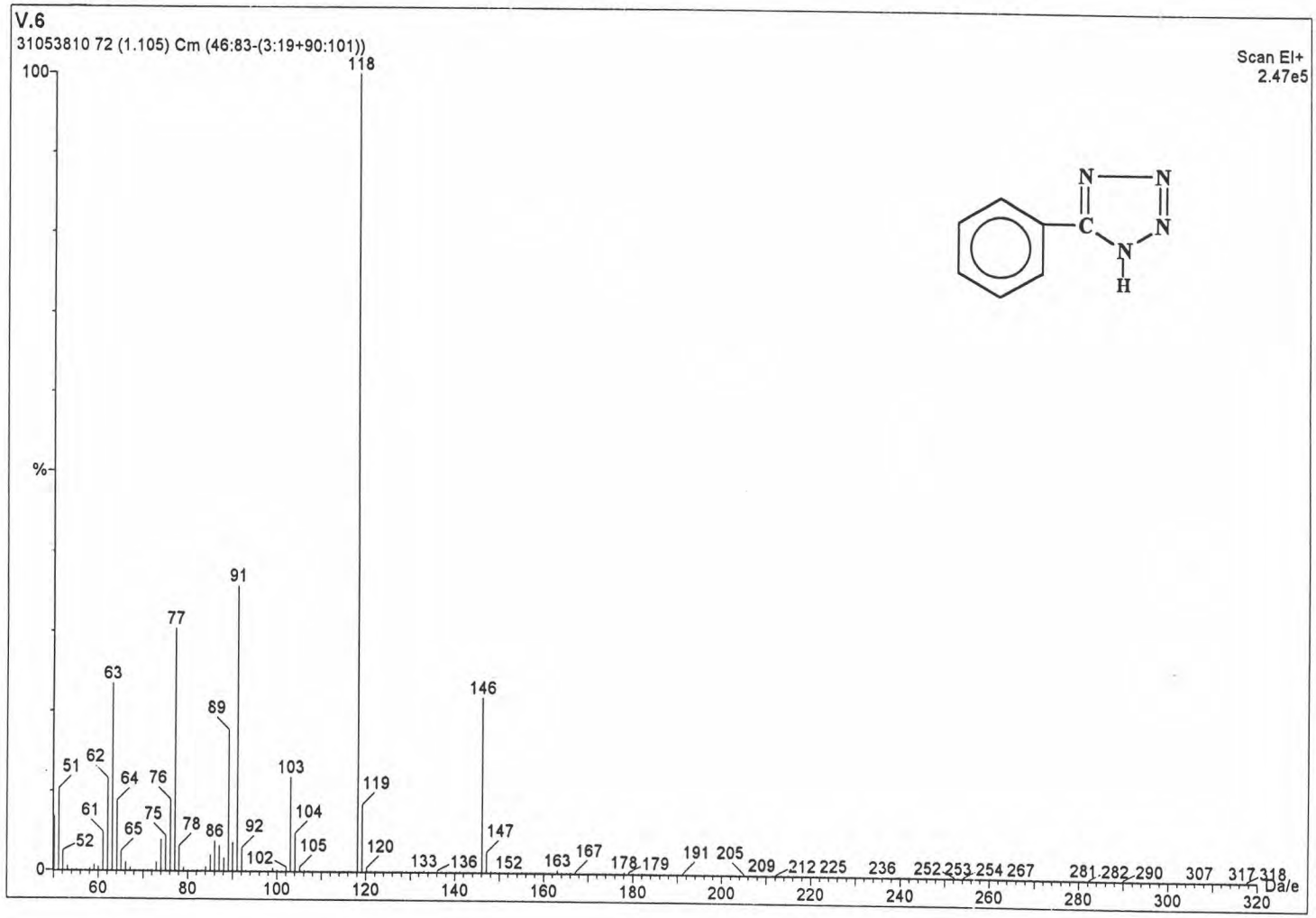

Figure A5 Mass spectrum of 5-phenyltetrazole

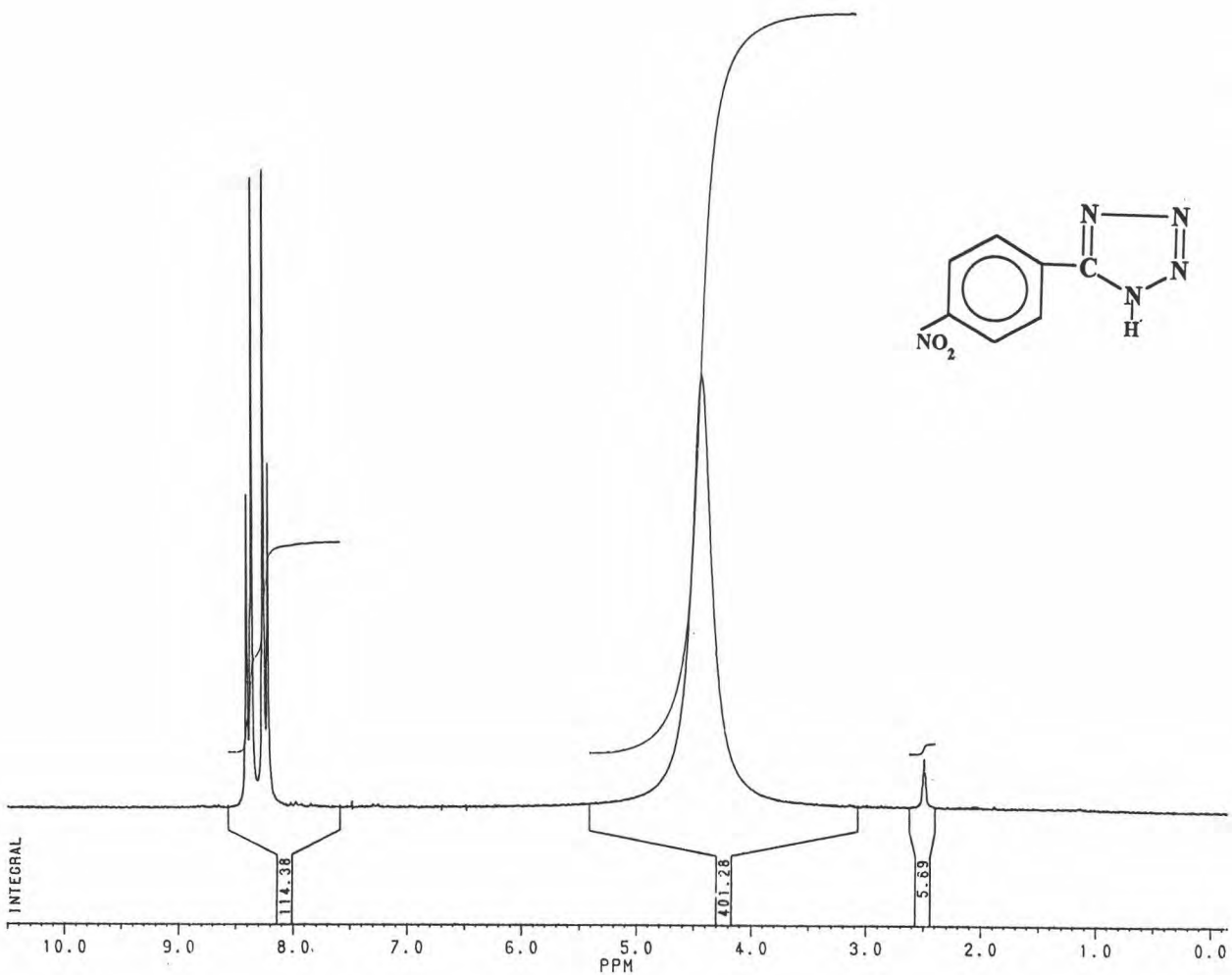

Figure A6 ^{1}H-NMR spectrum (DMSO-d_6) of 5-(4′-nitrophenyl)tetrazole

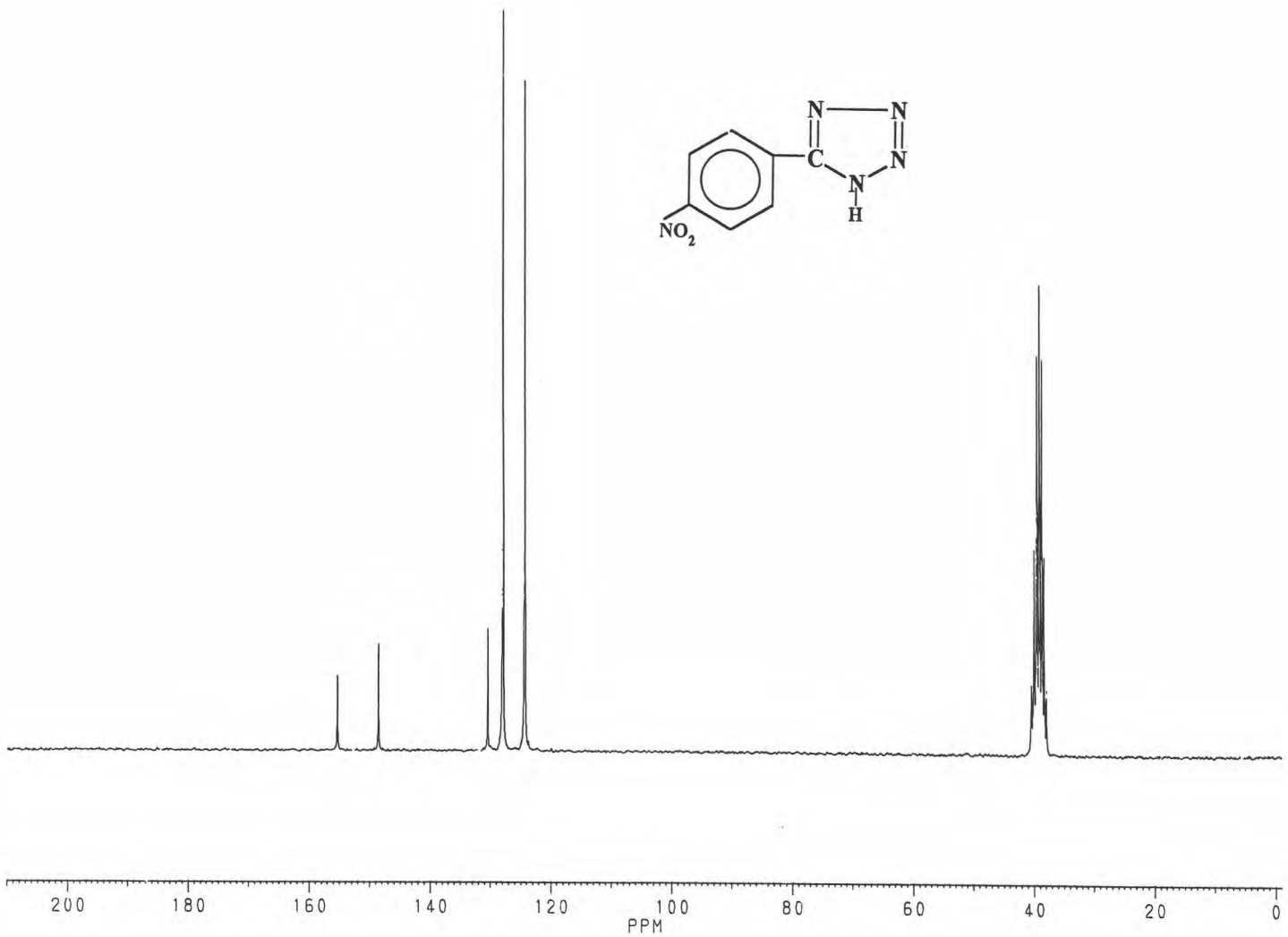

Figure A7 ^{13}C-NMR spectrum (DMSO-d_6) of 5-(4′-nitrophenyl)tetrazole

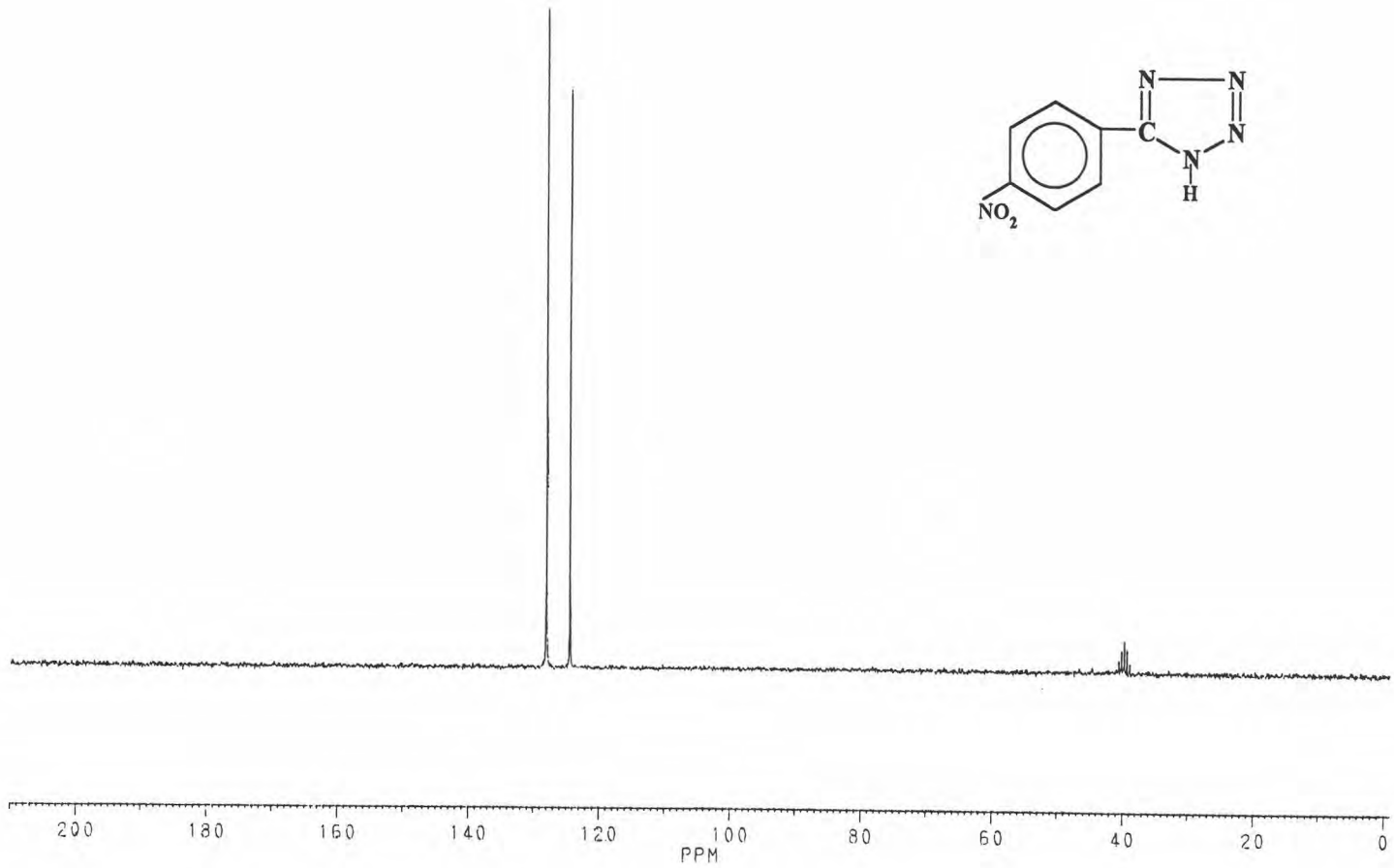

Figure A8 DEPT-90 ^{13}C-NMR spectrum (DMSO-d_6) of 5-(4′-nitrophenyl)tetrazole

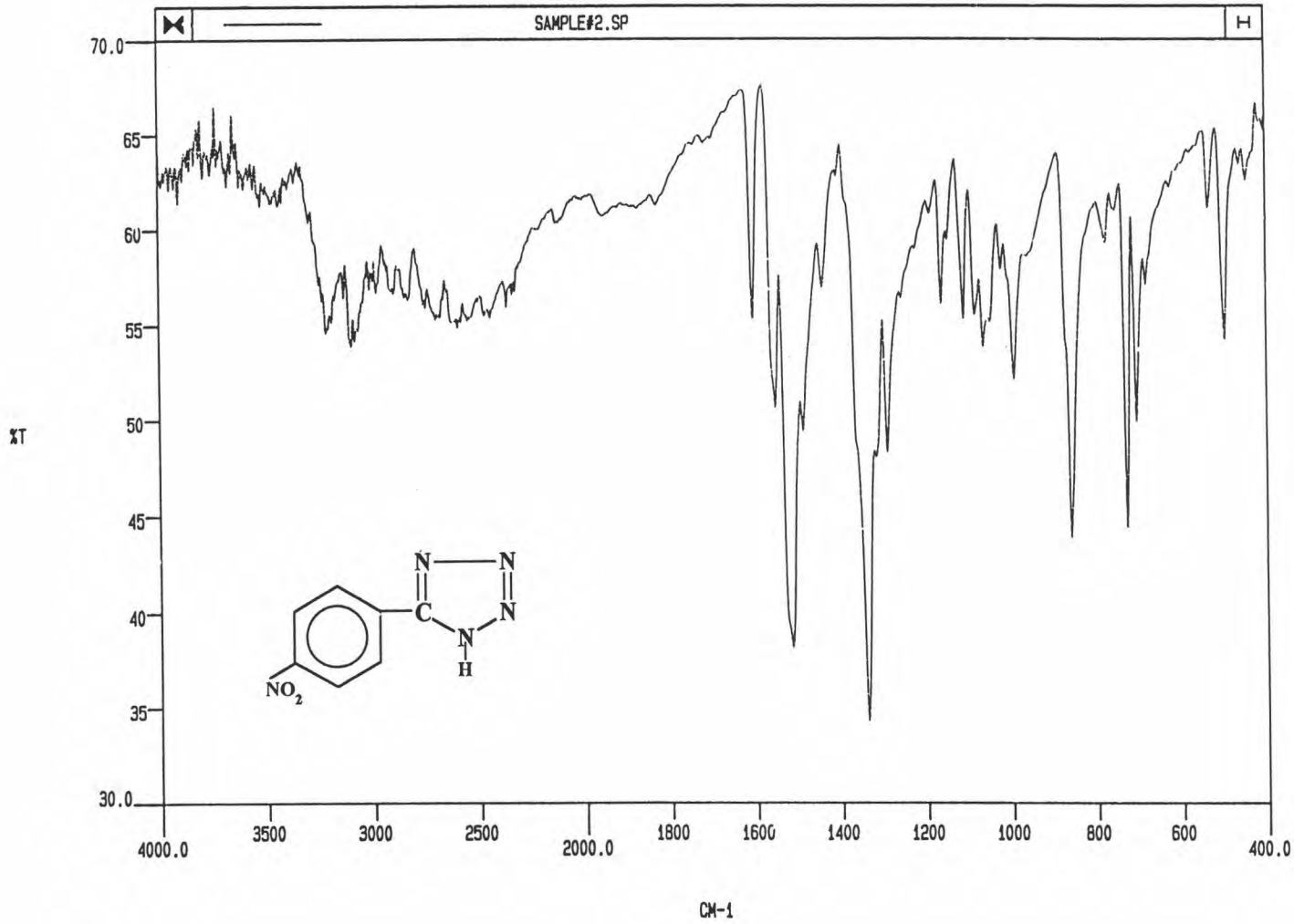

Figure A9 FTIR spectrum of 5-(4′-nitrophenyl)tetrazole

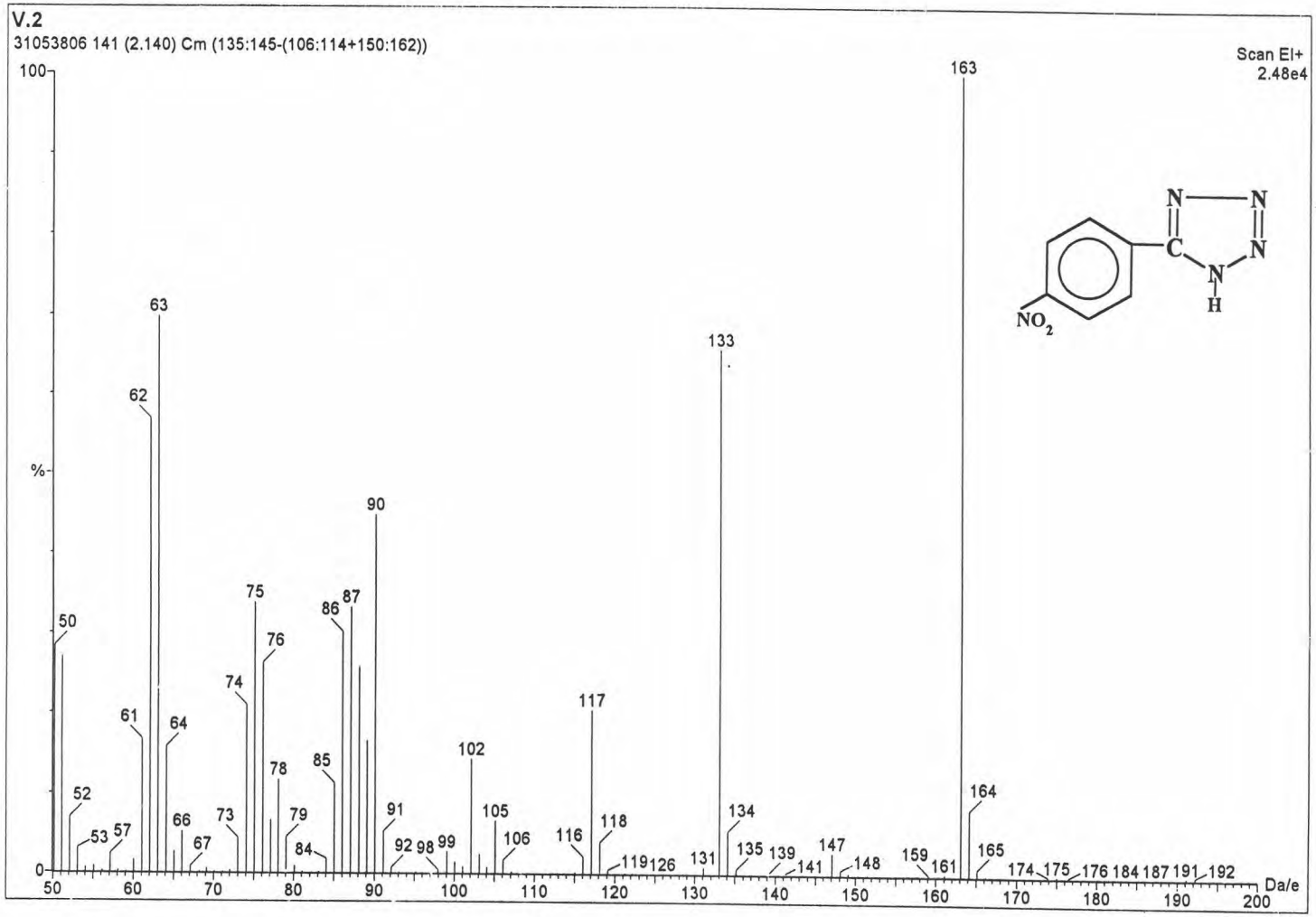

Figure A10 Mass spectrum of 5-(4′-nitrophenyl)tetrazole

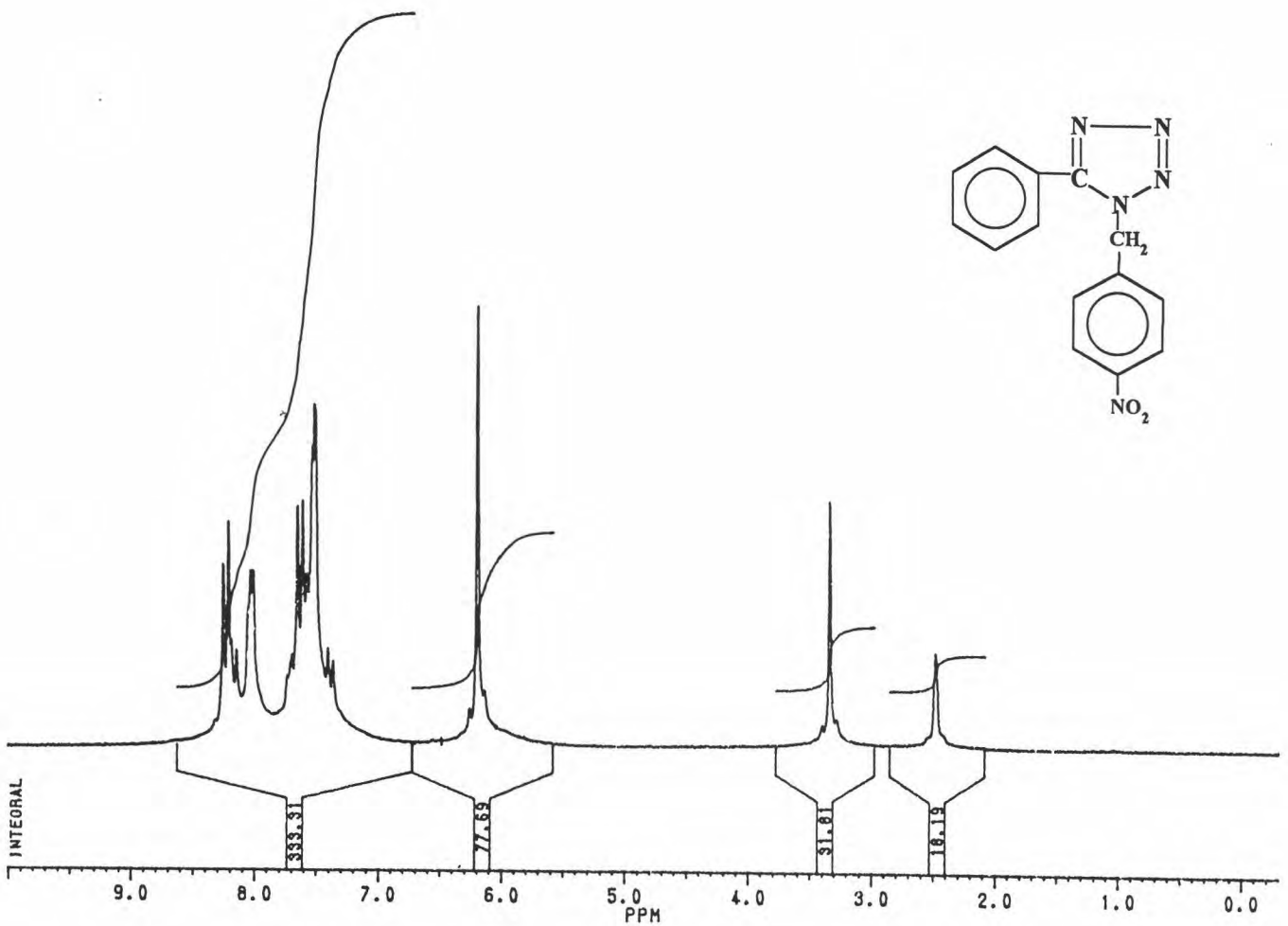

Figure A11 ^{1}H-NMR spectrum (DMSO-d_6) of 1-(4''-nitrobenzyl)-5-phenyltetrazole

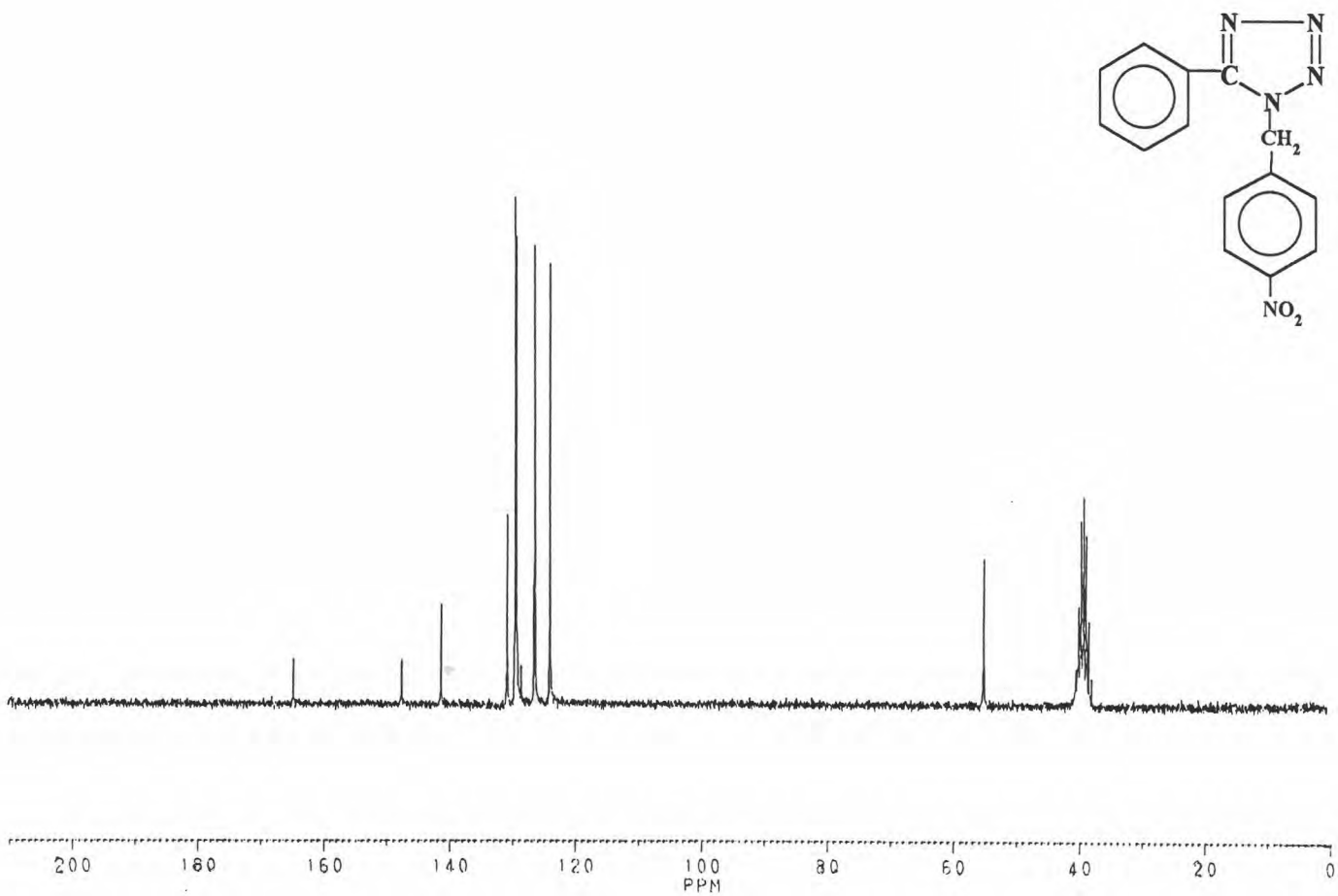

Figure A12 ^{13}C-NMR spectrum (DMSO-d_6) of 1-(4''-nitrobenzyl)-5-phenyltetrazole

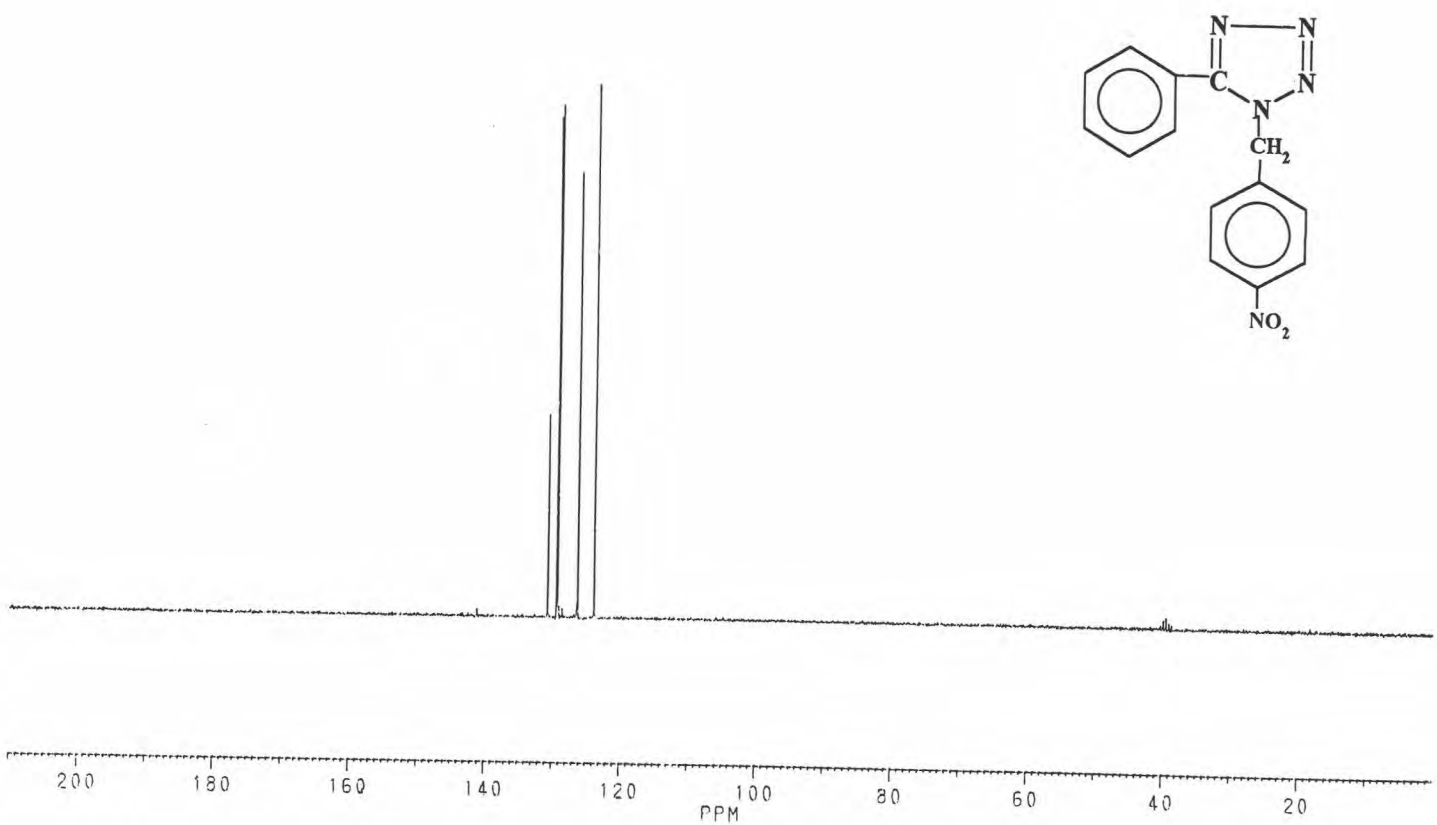

Figure A13 DEPT-90 ^{13}C-NMR spectrum (DMSO-d_6) of 1-(4''-nitrobenzyl)-5-phenyltetrazole

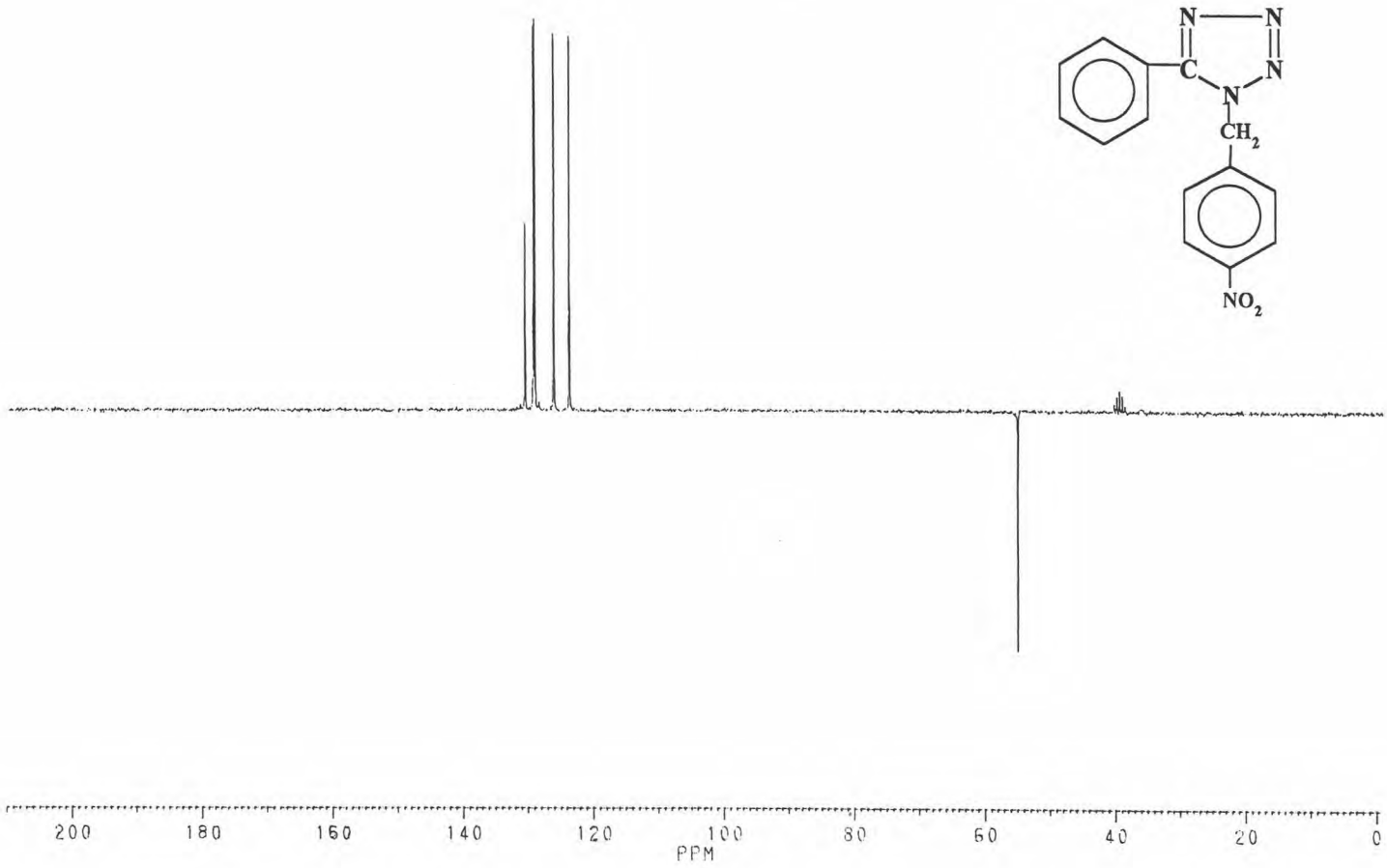

Figure A14 DEPT-135 ^{13}C-NMR spectrum (DMSO-d_6) of 1-(4''-nitrobenzyl)-5-phenyltetrazole

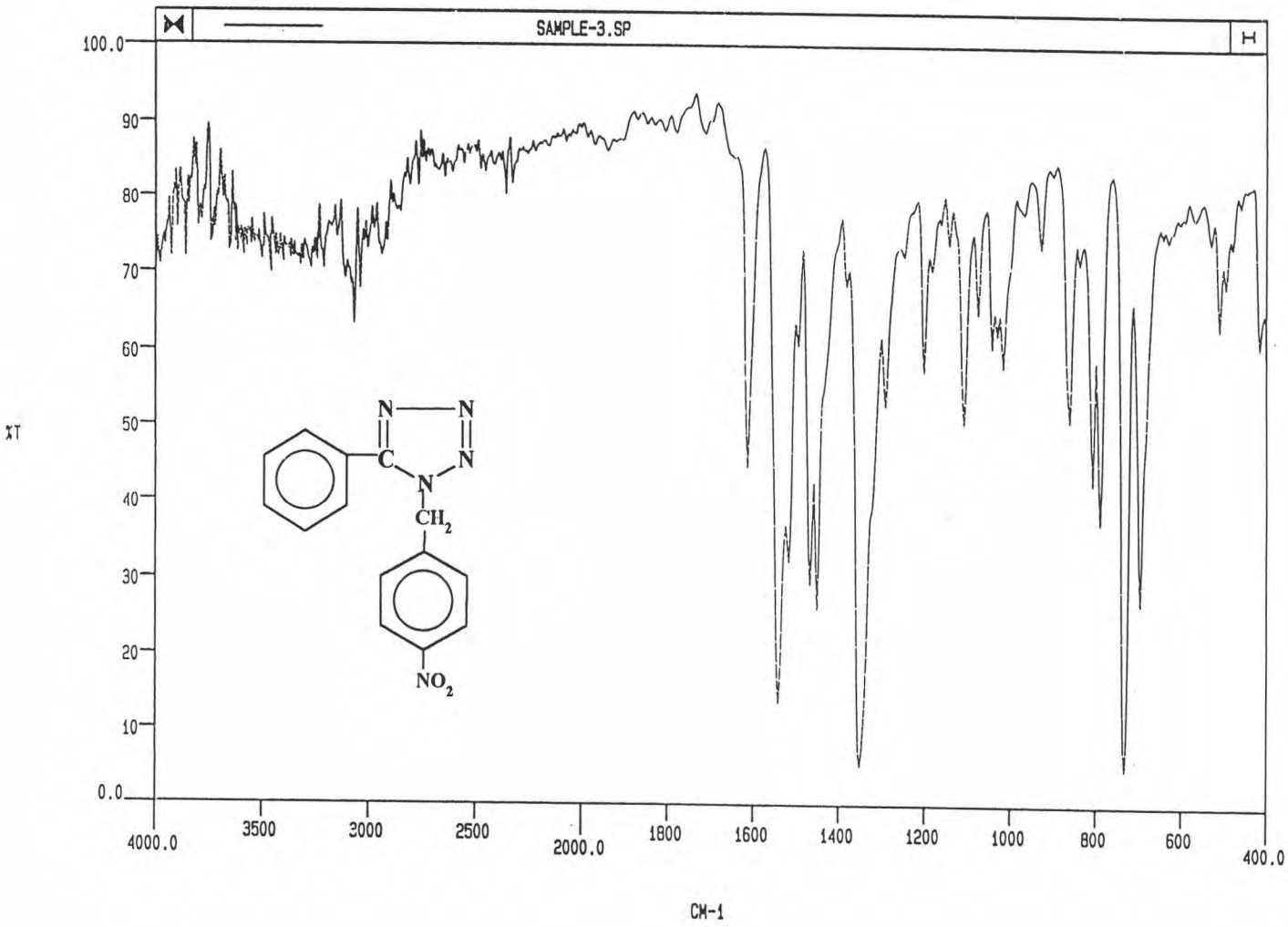

Figure A15 FTIR spectrum of 1-(4′′-nitrobenzyl)-5-phenyltetrazole

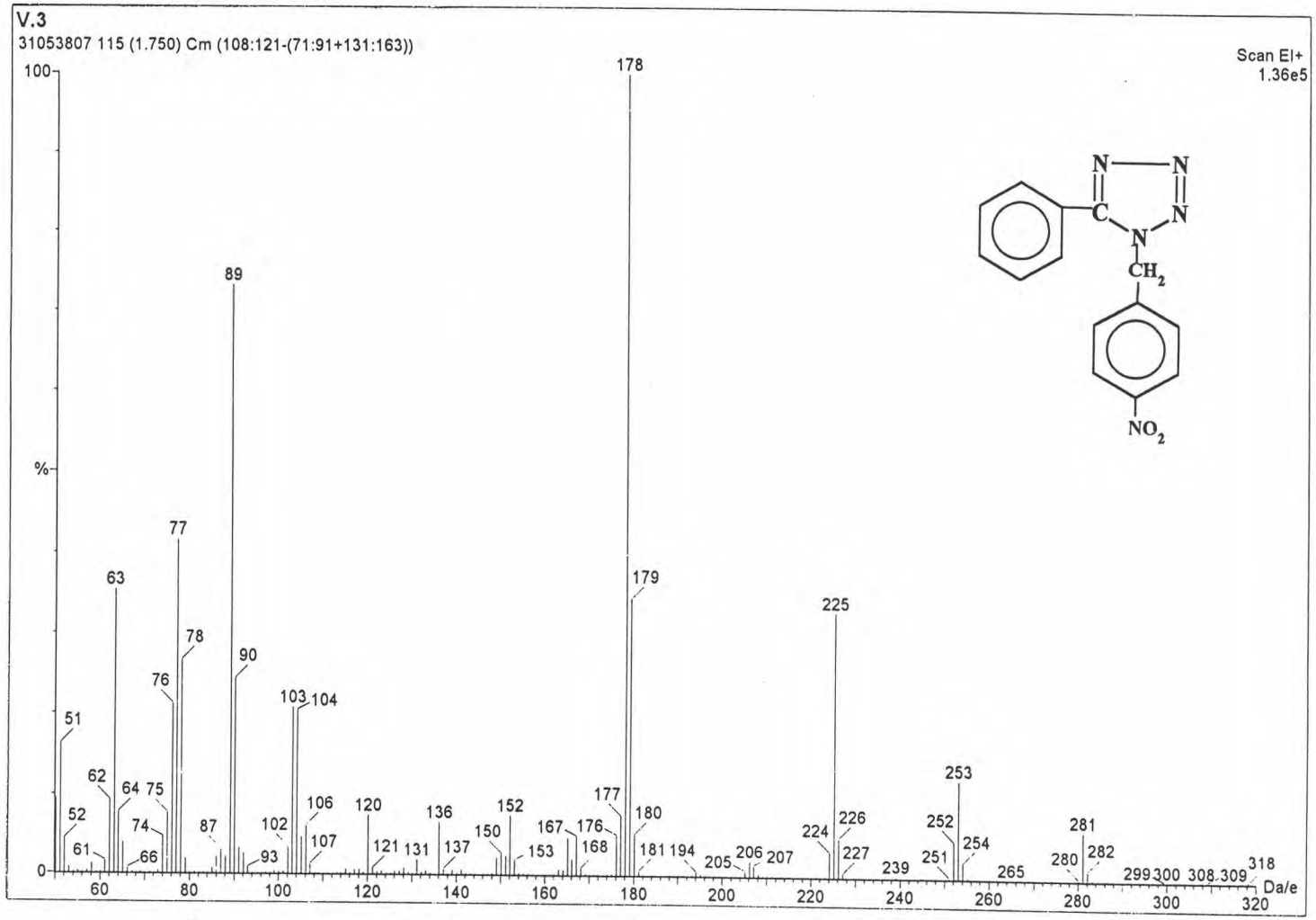

Figure A16 Mass spectrum of 1-(4''-nitrobenzyl)-5-phenyltetrazole

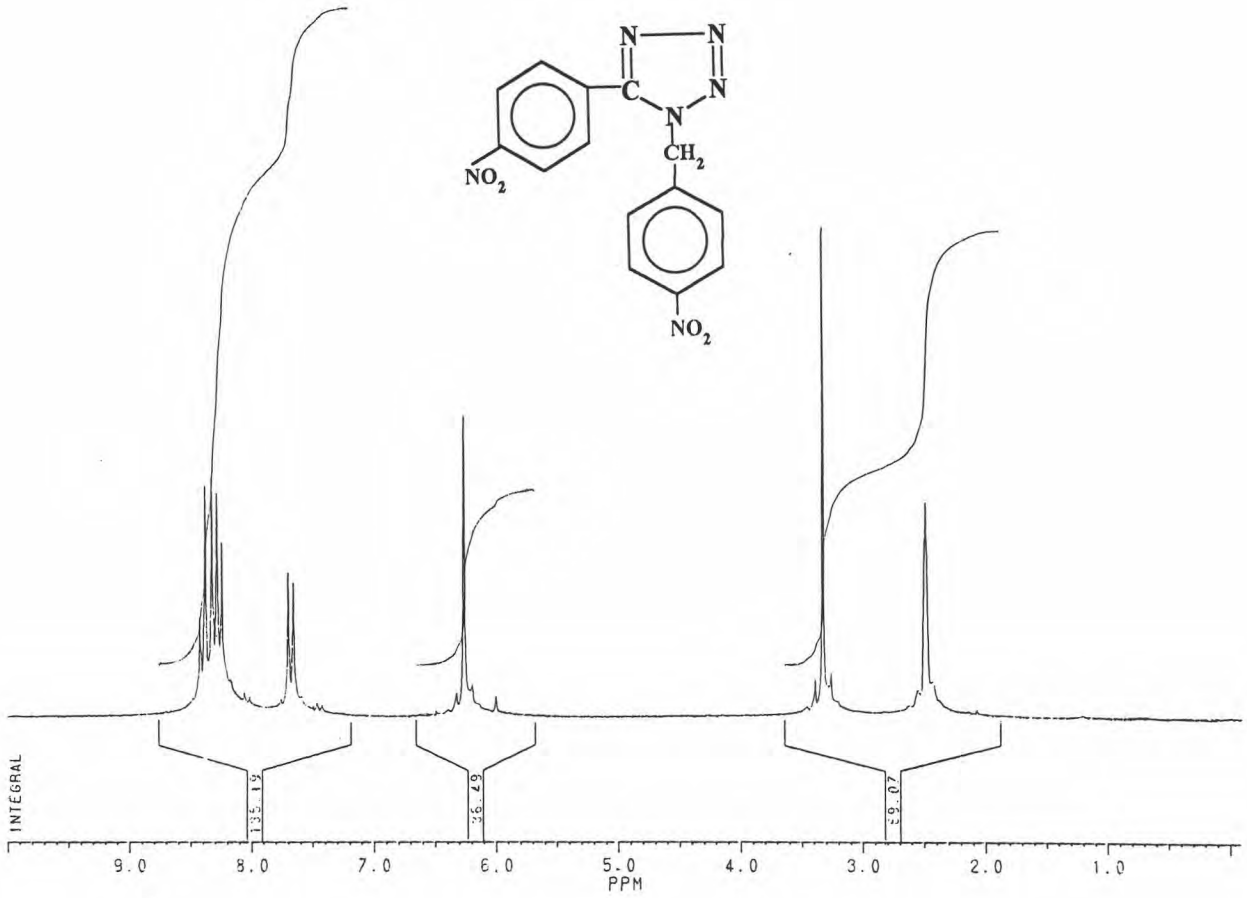

Figure A17 ^{1}H-NMR spectrum (DMSO-d_6) of 1-(4″-nitrobenzyl)-5-(4′-nitrophenyl)tetrazole

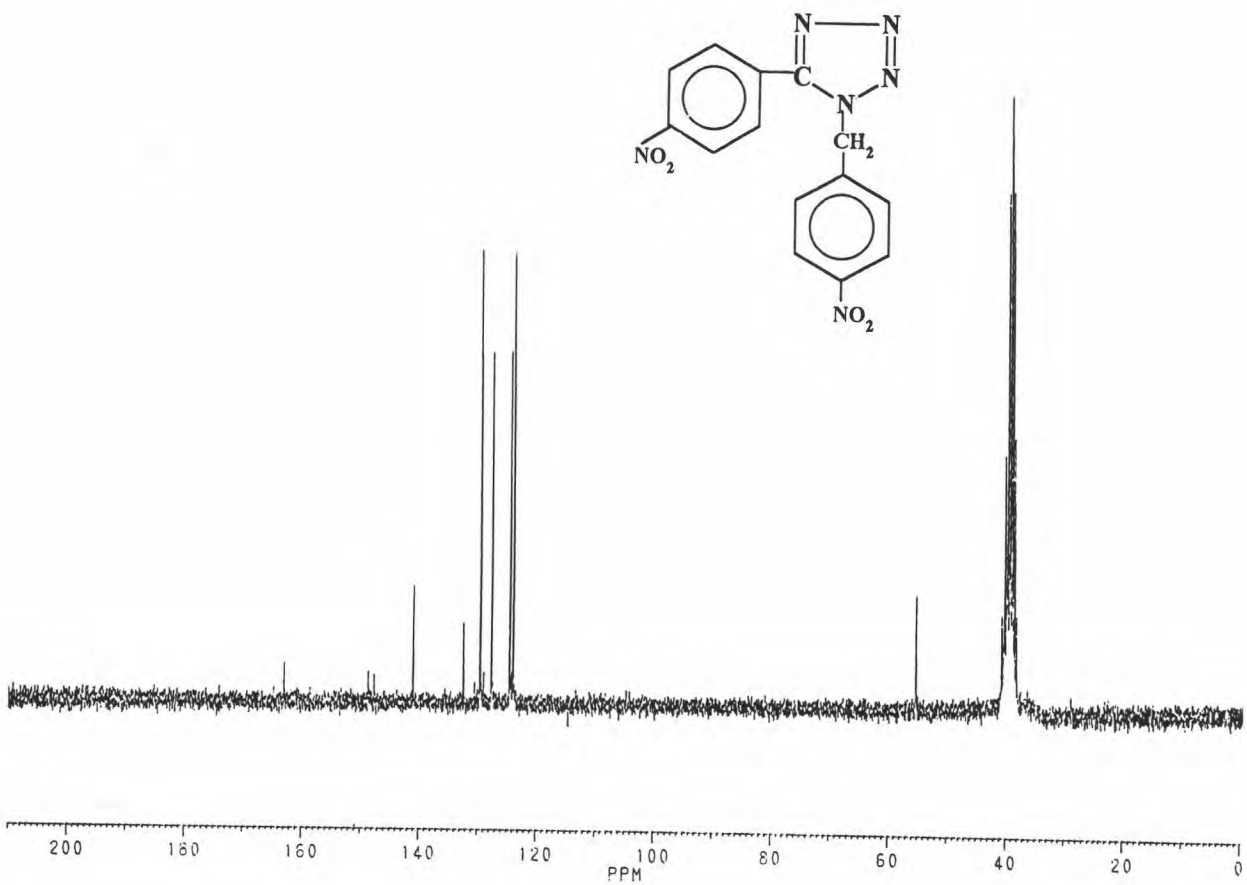

Figure A18 ^{13}C-NMR spectrum (DMSO-d_6) of 1-(4''-nitrobenzyl)-5-(4'-nitrophenyl)tetrazole

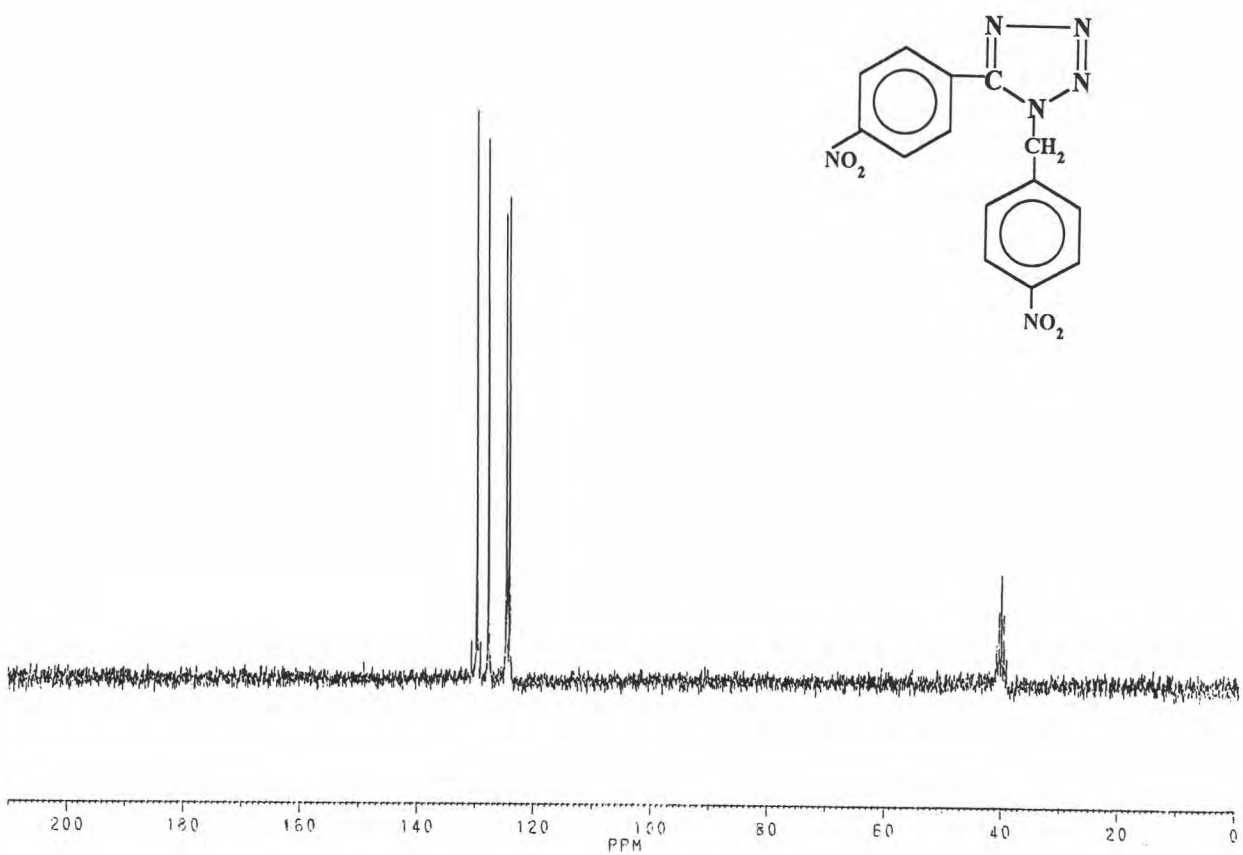

Figure A19 DEPT-90 ^{13}C-NMR spectrum (DMSO-d_6) of 1-(4′′-nitrobenzyl)-5-(4′-nitrophenyl)tetrazole

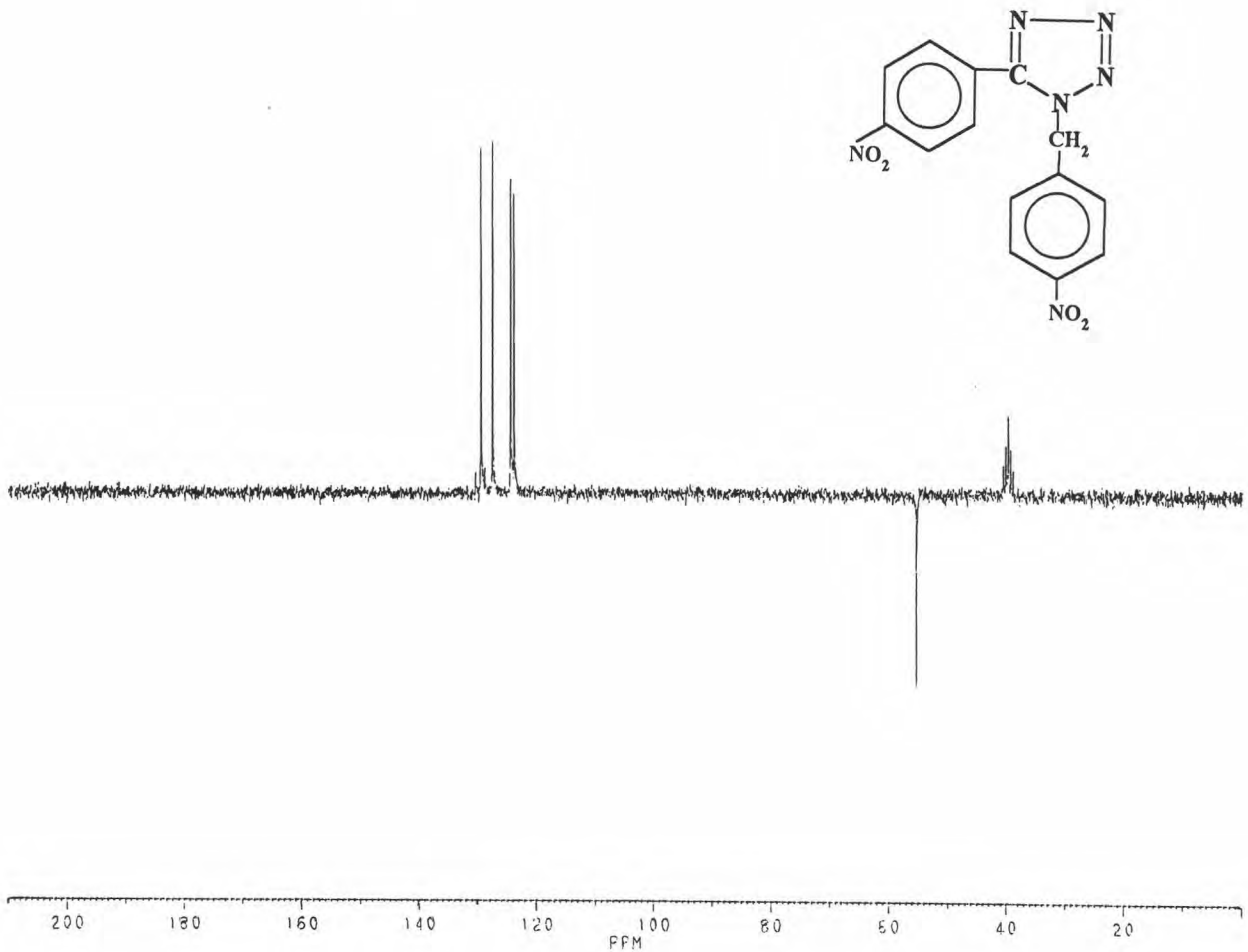

Figure A20 DEPT-135 ^{13}C-NMR spectrum (DMSO-d_6) of 1-(4''-nitrobenzyl)-5-(4'-nitrophenyl)tetrazole

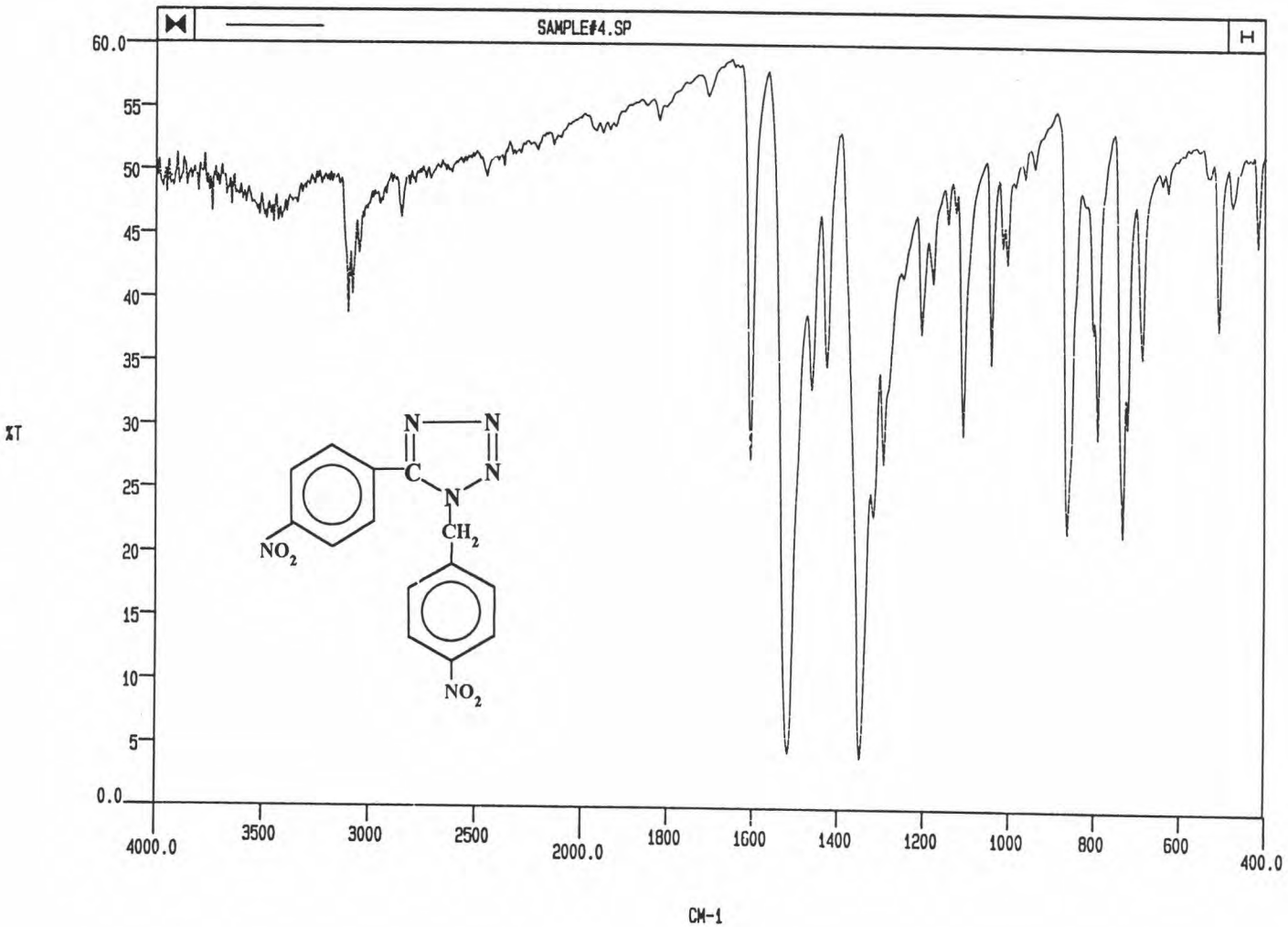

Figure A21 FTIR spectrum of 1-(4′′-nitrobenzyl)-5-(4′-nitrophenyl)tetrazole

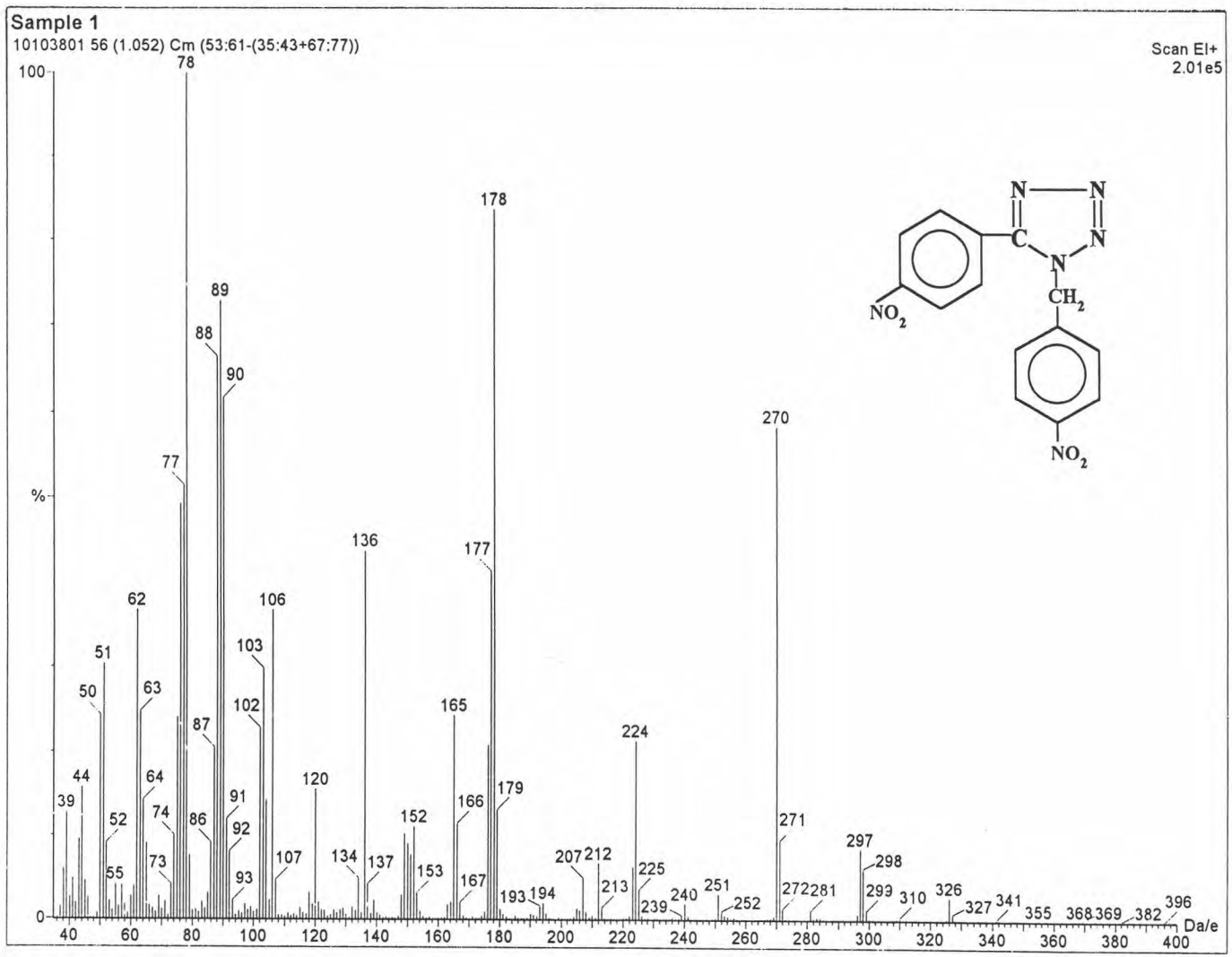

Figure A22 Mass spectrum of 1-(4′′-nitrobenzyl)-5-(4′-nitrophenyl)tetrazole

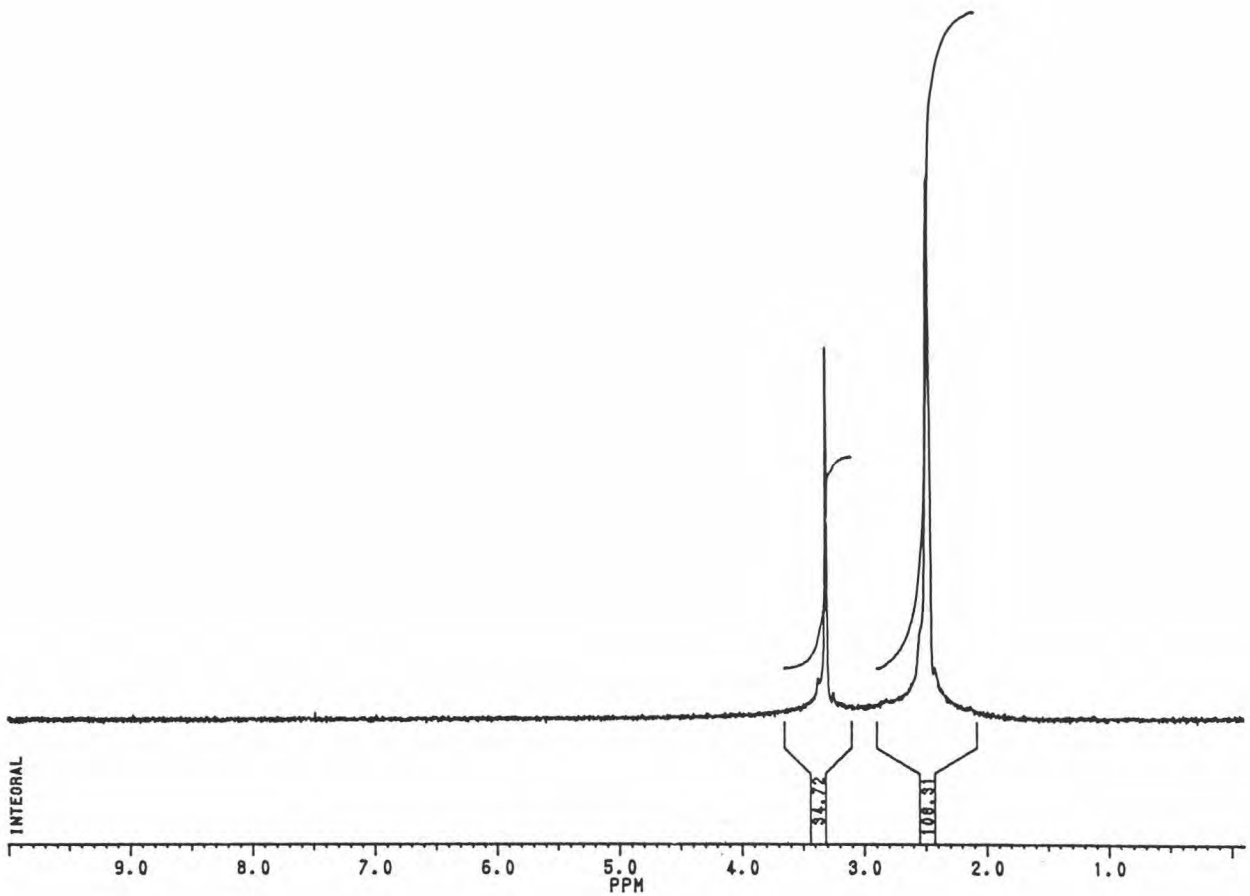

Figure A23 ^{1}H-NMR spectrum of dimethylsulfoxide-d_6 (DMSO-d_6)

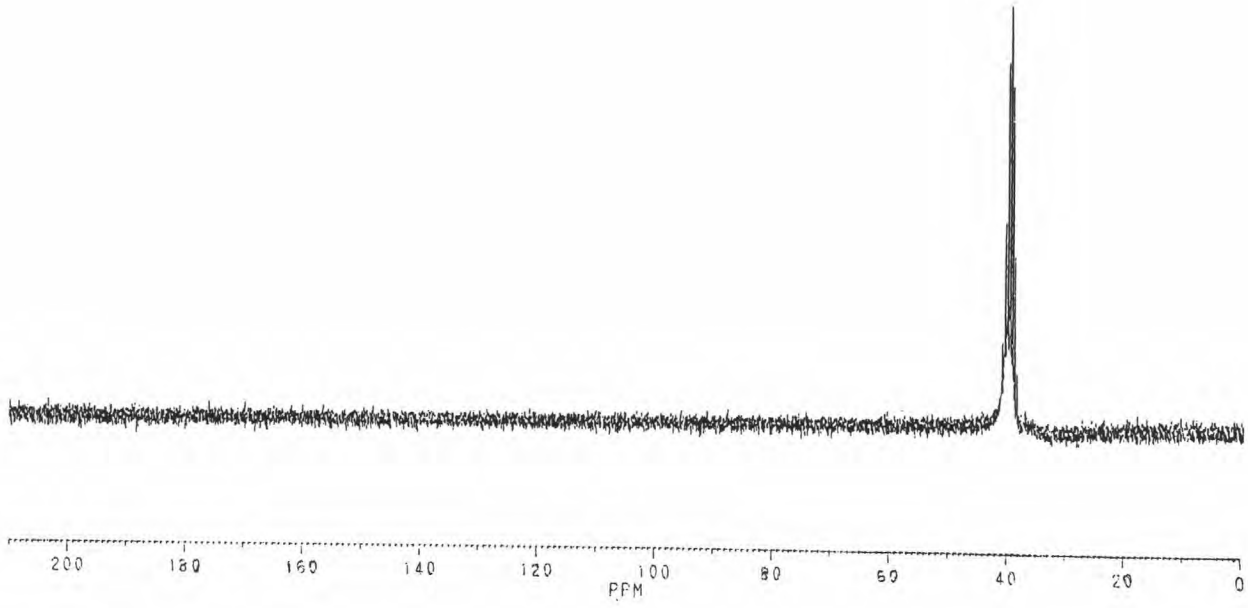

Figure A24 ^{13}C-NMR spectrum of dimethylsulfoxide-d_6 (DMSO-d_6)

APPENDIX B

^{13}C-NMR Spectrometry for Diesel Fuel

^{13}C-NMR method is one of the most important features in separation of paraffinic, naphthenic and aromatic carbon percentages. All the accurate result of carbon types can be directly observed by this technique. Figure B1 is ^{13}C-NMR spectrum of base diesel fuel. [19]

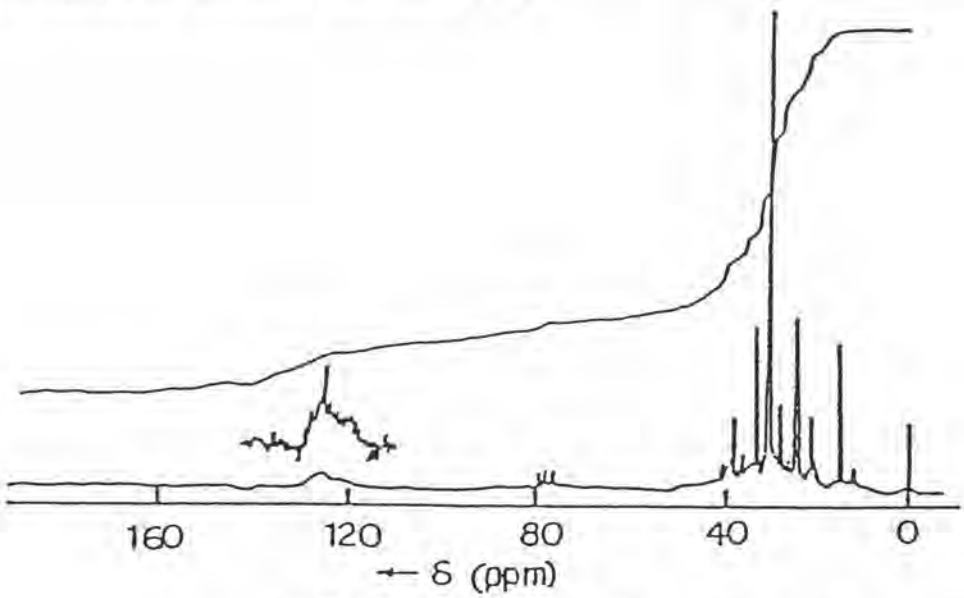

Figure B1 ^{13}C-NMR spectrum of base diesel fuel

In the calculation, the percentage of aromatic carbon was obtained by summation of the intensities from 110 to 160 ppm diveded by total integrated area (excluding the area of solvent), while the percentage of the paraffinic carbon was calculated in similar manner but involving only the intensities from 0-25 ppm and the resolved intensities from 25-60 ppm.

Since %Cp + %Cn + %Ca = 100 , the percentage of the naphthenic carbon, %Cn, can be obtained by difference.

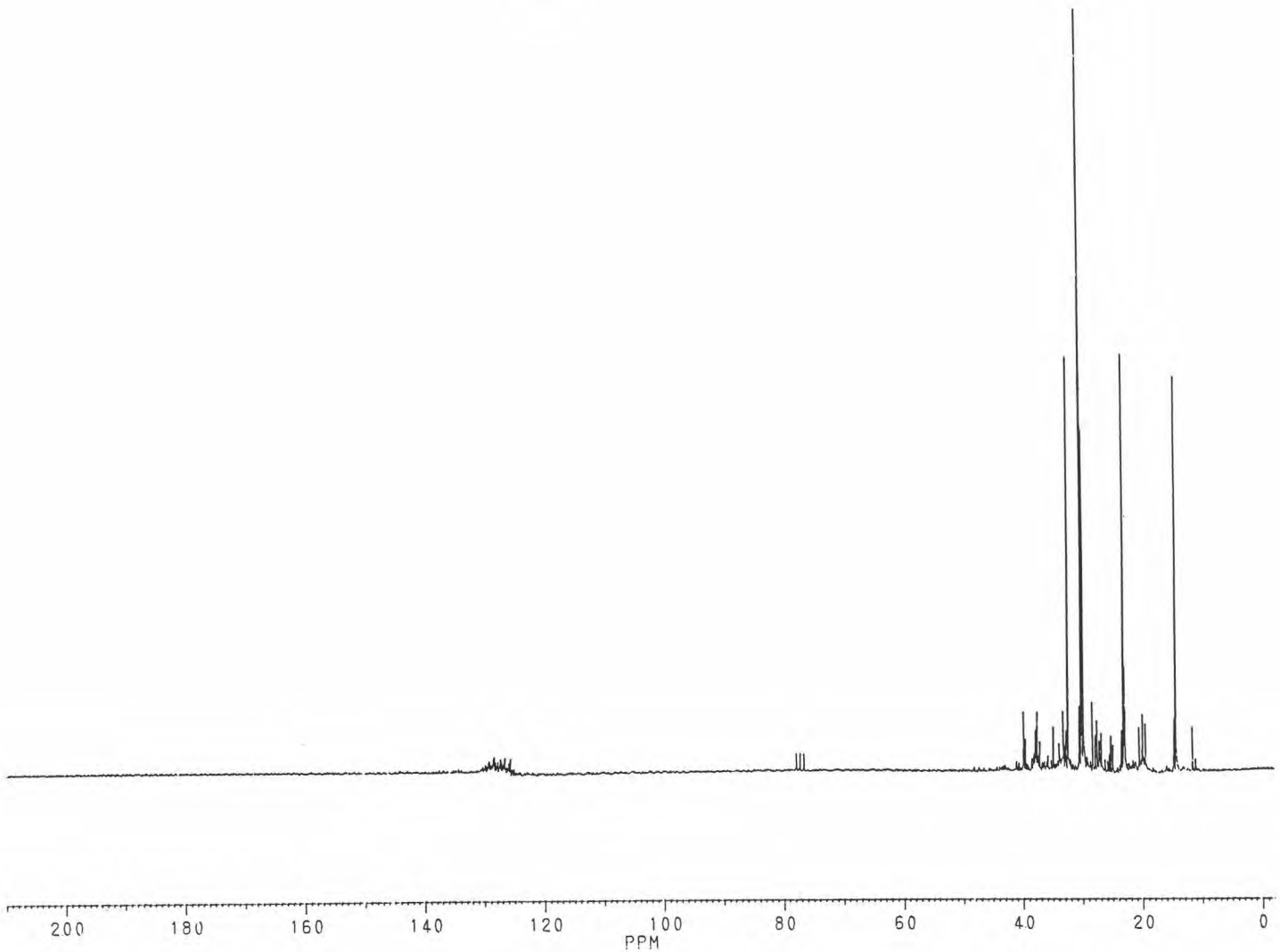

Figure B2 ^{13}C-NMR spectrum ($CDCl_3$) of base diesel fuel

APPENDIX C

Properties of base diesel fuel (high speed diesel, 338)

Properties	Test Method	Limits	Results
API Gravity @ 60 °F	ASTM D1298	report	35.5
Specific Gravity @ 15.6/15.6 °C	ASTM D1298	0.81-0.87	0.8437
Calculated Cetane Index	ASTM D976	47 min	48.75
Cetane Number	ASTM D613	min	-
Kinematic Viscoscity			
@ 40 °C (104 °F), cSt	ASTM D445	1.8-4.1	2.7991
Pour Point, °C	ASTM D97	10 max	-18
Sulphur Content, % wt	ASTM D129	0.5 max	0.175
Copper Strip Corrosion			
(3 hrs @ 50 °C)	ASTM D130	No.1 max	-
Conradson Carbon Residue, % wt	ASTM D189	0.05 max	-
Water & Sediment, % vol.	ASTM D2709	0.05 max	traces
Ash, % wt	ASTM D482	0.01 max	-
Flash Point, °C	ASTM D93	66 min	73
Distillation, °C	ASTM D86		
Initial Boiling Point		report	177
10 % vol evaporated		report	217
50 % vol evaporated		report	270
90 % vol evaporated		338 max	317
Color, ASTM	ASTM D1500	4.0 max	2.5

APPENDIX D

THE CALCULATION OF CETANE INDEX

The Calculated Cetane Index is determined from the following equation:

1. When it is not applicable to fuels containing additives for raising cetane number.

$$\text{Calculated cetane index} = -420.34 + 0.016G^2 + 0.192G \log M + 65.01 (\log M)^2 - 0.0001809 M^2 \quad (1)$$

2. When it is applicable to fuels containing additives for raising cetane number. The Calculated Cetane Index is determined from the equation 1 plus equation 2

$$\text{Improver value} = 0.1742(0.1G)^{1.4444} (0.1M)^{1.0052} \{\ln(1+17.5534D)\} \quad (2)$$

where

G = API gravity, determined by Test Method D287 or D 1298,

M = mid-boiling temperature, °F, determined by Test Method D86 and corrected to standard barometric pressure.

D = percent weight of cetane improver, % wt.

For example

1. Determine the cetane index of diesel base fuel from equation 1 when mid-boiling point at 518 °F, API gravity = 35.5

Solution

From equation 1, the calculated cetane index is

Calculated cetane index = $- 420.34 + 0.016G^2 + 0.192G \log M +$
$65.01 (\log M)^2 - 0.0001809 M^2$

Hence the calculated cetane index is

$= - 420.34 + 0.016(35.5)^2 + 0.192(35.5)\log (518)$
$+ 65.01 (\log (518))^2 - 0.0001809 (518)^2$

Calculated cetane index = 48.75

2. Determine the calculated cetane index improver, when the blended of diesel base fuel with tetrazole derivatives and 2.5 %V hexanol.

When mid-boiling point at 514.4°F, API gravity = 35.7 and tetrazole derivatives as 0.05 %wt.

Solution

From equation 1, the calculated cetane index is

$= - 420.34 + 0.016(35.7)^2 + 0.192(35.7)\log (514.4)$
$+ 65.01(\log (514.4))^2 - 0.0001809 (514.4)^2$

Calculated cetane index = 48.67

From equation 2 the improver value is

Improver value = $0.1742(0.1G)^{1.4444} (0.1M)^{1.0052} \{\ln(1+17.5534D)\}$

Hence

$= 0.1742(0.1(35.7))^{1.4444} (0.1(514.4))^{1.0052}$
$\{\ln(1+17.5534(0.05))\}$

Improver value = 3.58

Calculated cetane index improver = calculated cetane index + improver value

Hence

$= 48.67 + 3.58$

Calculated cetane index improver = 52.25

VITA

Wichit Rattanatawonkiti was born on June 6, 1970 in Prachuapkhirikhan, Thailand. He recived his Bachelor's Degree of Science in Industrial Chemistry, Chiang Mai University in 1993. He continued his Master's study at Chulalongkorn University in 1993 and finished in 1996.